ABSTRACT

This research studies the effect of replacing hydrogen atom with deuterium (monodeuteriation) on the stability of trans-HCOH using density functional theory. The study begins by verifying that the monodeuteriation does not affect the electronic structure, but it does the vibrational frequency of the molecule. The potential barrier function is predicted using intrinsic reaction coordinate calculation and it is used to calculate the quantum tunneling probability using Wentzel-Kramers-Brillouin (WKB) approximation. The results demonstrate that the monodeuteration decreases the molecule's vibrational frequency as well as the quantum tunneling probability. The half-life calculation after monodeuteration is 2.97×10^{16} hours, which is extremely longer than before monodeuteration that is only 2.5 hours using the same calculation methods. As the supplementary results, this research investigates the monodeuteriation effect on H_2 and H_2O and analyzes the reason of using trans-HCOD instead of trans-DCOH in experiment done by Schreiner *et al*.

Keyword: monodeuteriation, density functional theory, quantum tunneling, WKB approximation